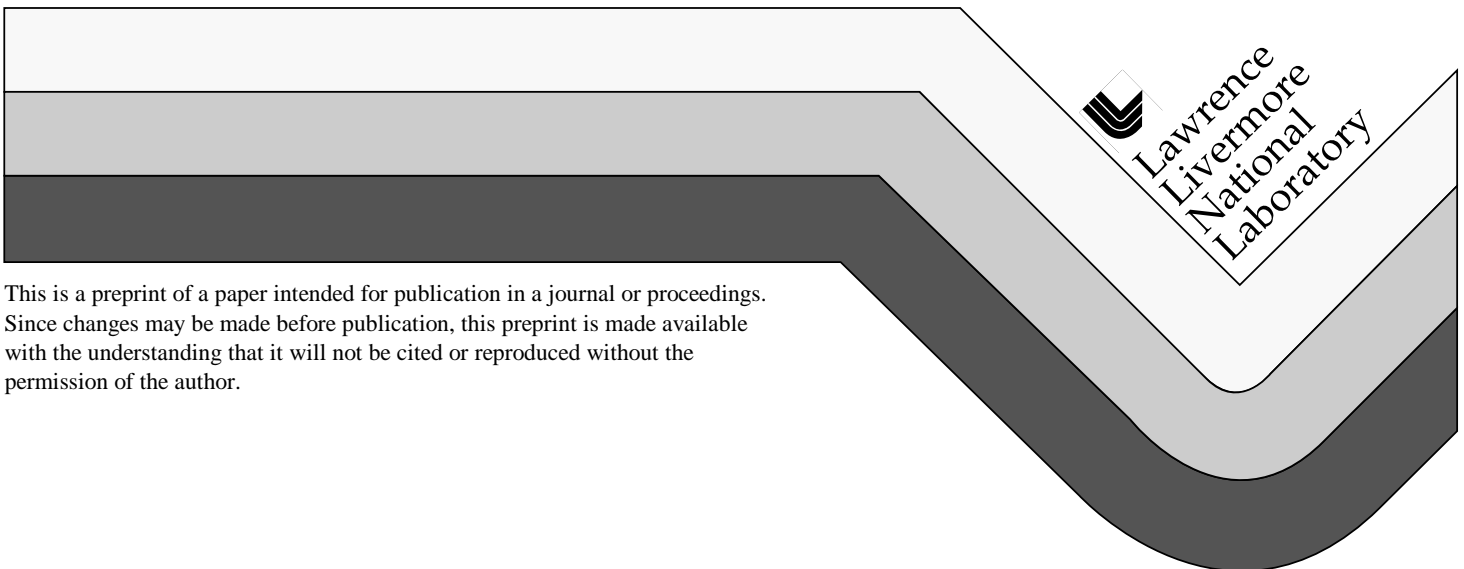# A Crystal Level Model for Phase Transformation Allowing for Large Volume Changes

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A CRYSTAL LEVEL MODEL FOR PHASE TRANSFORMATION ALLOWING FOR LARGE VOLUME CHANGES

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ABSTRACT: We present a model for materials undergoing diffusionless structural changes including martensitic phase transformation and twinning, with the phase transformations involving large volume changes. Within a given material element, structural changes induce mass fraction rates between the constituents in the material. Deformation results from both these structural changes and elasto-viscoplastic deformation of the constituents themselves.

INTRODUCTION: We are interested in structural changes occuring during deformation driven scenarios, and seek to model situations in which material deforms considerably after undergoing structural change. In the model outlined here, transformation induces mass fraction rates among the constituents making up the material element and a linking assumption is used to partition deformation among the constituents. A multiplicative decomposition of the deformation gradient is used within each constituent, and the constituent response follows a large strain crystal elasto-viscoplasticity model. Plastic deformation of the constituents is associated with slip system activity. Strains resulting from structural changes may be accommodated by elastic and plastic deformation of the constituents and by further phase transformation or twinning modes. The model has been implemented for FCC twinning and for FCC to BCC martensitic transformation. Results are shown for homogeneous deformations. Finite element simulation results have also been obtained, but are not presented here due to space restrictions.

Several other assumptions help to keep the formulation tractable. All constituents have the same Cauchy stress and the spin is partitioned so that lattice orientation correspondences of the structural changes are preserved. Dislocation density state variables describe material hardening, and dislocation density is assumed to be carried through structural changes. And finally we assume that structural changes are not nucleation limited and that we need not consider site potency distributions.

METHODS, RESULTS, AND DISCUSSION: At a given location, the state of the material is described by a single orientation, the Cauchy stress, the mass fractions of the constituents, and the dislocation density in each of the constituents. Because the constituents

rotate together, the orientation correspondences between them are fixed and a single reference orientation may be used to describe orientations of all of the constituents. Similarly, elastic stretches in all of the variants may be determined from the single Cauchy stress. More elaborate linking assumptions could be used among the constituents, with the possible introduction of more variables to describe the state of the material. The increased complexity would most likely entail additional assumptions regarding microstructural morphology or additional descriptors related to the morphology. Both of these additions are avoided by the simple linking assumption employed here. Resolution of the microstructure to the scale of individual transformed domains would reduce the impact of any linking assumption and modifications of the model for this purpose may be considered in future work.

See Figure 1(a) for a schematic of the kinematics. Given the current volume fractions v^α, the total apparent velocity gradient has the form $\langle \mathbf{L} \rangle = \mathbf{L}^{\chi_*} + \sum_\alpha v^\alpha \mathbf{L}^\alpha$, with $\mathbf{L}^{\chi_*} = \sum_i \mathbf{L}^{i_\alpha^\beta}$ and with $\mathbf{L}^\alpha$ being the velocity gradient within constituent α. The velocity gradient contributions due to structural change modes have the form

$$\mathbf{L}^{i_\alpha^\beta} = \dot{m}^{i_\alpha^\beta} \left[\frac{a^\beta}{a^\alpha} \mathbf{V}^\beta \cdot \hat{\mathbf{G}}^{i_\alpha^\beta} \cdot (\mathbf{V}^\alpha)^{-1} + \frac{a^\beta}{a^\alpha} \mathbf{V}^\beta \cdot (\mathbf{V}^\alpha)^{-1} - \mathbf{I} \right] \tag{1}$$

with $\dot{m}^{i_\alpha^\beta}$ being the associated mass fraction rate. The tensor $\hat{\mathbf{G}}^{i_\alpha^\beta}$ captures the deformation associated with the structural change and it must be augmented due to the deformations of the constituents. Elastic stretch and isotropic thermal expansion of the constituents are captured by the $\mathbf{V}^\alpha$ and a^α respectively. The driving force for structural changes includes terms arising from mechanical work, from the temperature dependent chemical free energy change on transformation, and from interaction energy among the constituents:

$$f^{i_\alpha^\beta} = f_d^{i_\alpha^\beta} - C^{\chi_\alpha^\beta} \cdot (\theta - \theta_o^{\chi_\alpha^\beta}) + f_r^{\chi_\alpha^\beta}(m^\eta). \tag{2}$$

The driving force contribution due to mechanical work involves $\boldsymbol{\tau}^\alpha$, the Kirchhoff stress in constituent α, and takes the form

$$f_d^{i_\alpha^\beta} = \boldsymbol{\tau}^\alpha : \left(a^\beta \mathbf{V}^\beta \cdot \hat{\mathbf{F}}^{\chi_\beta} \cdot (\hat{\mathbf{F}}^{\chi_\alpha})^{-1} - a^\alpha \mathbf{V}^\alpha \right). \tag{3}$$

The form of the interaction forces $f_r^{\chi_\alpha^\beta}$ depends on the system under consideration and details are omitted. The kinetics for both dislocation glide and structural change follow a power law form. See Ghosh and Olson [1994] for a discussion of the similarities between the kinetics for slip and for phase transformation when phase transformation is in the thermally activated regime.

FCC to BCC martensitic transformation follows the Bain distortion and produces three variants, as in Artemev et al. [2001]. Coupled thermo-mechanical effects can be important, but such results are not included here. Figure 1(b) demonstrates that the model can produce
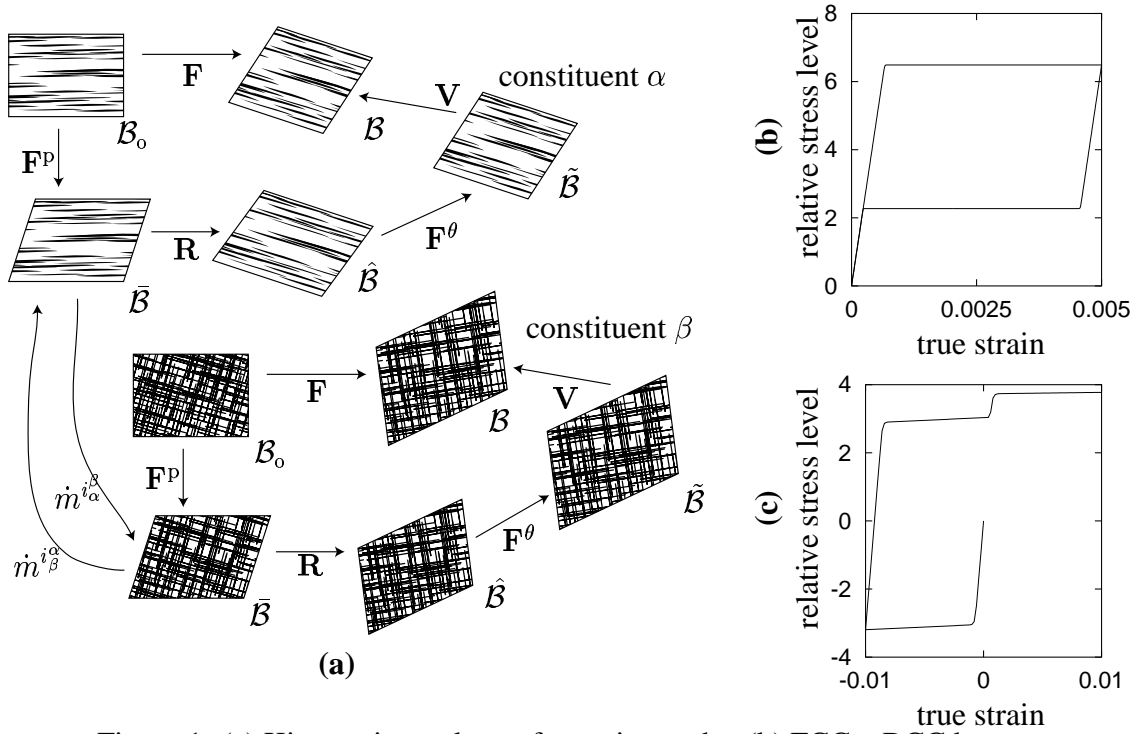
Figure 1: (a) Kinematics and transformation paths; (b) FCC↔BCC hysteresis loop; (c) compression-tension for twinning material.

the well know flag-type hysteresis loop under isothermal conditions above the reference temperature for the transformation ($\theta_o^{\chi_\alpha^\beta}$). Such behavior is of importance in shape memory alloys (Huo and Muller [1993]).

FCC twinning results are shown in Figure 1(c). Relatively small strains are used in the depicted reverse loading scenario so that elastic transients are clear. Compression twins are formed and revert to the parent constituent on reverse loading. Tensile twins do not form because they are not oriented as favorably and the material deforms by dislocation glide before tensile twinning is activated.

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